12, March 2013, NR/HEP^2 @ Instituto Superior Técnico

Initial Conditions
for Numerical Relativity

∼ Introduction to numerical methods for solving elliptic PDEs ∼

Part II

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Introduction

Overview of 2nd order PDEs

- Second order PDE

$$A\frac{\partial^2 u}{\partial t^2} + 2B\frac{\partial^2 u}{\partial t \partial x} + C\frac{\partial^2 u}{\partial x^2} + f(t,x) = 0$$

Numerical Cost

$B^2 - AC < 0$: Elliptic type $\triangle \psi = 0$
(Laplace equation, etc.)

$B^2 - AC = 0$: Parabolic type $\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2}$
(Heat conduction equation, etc.)

$B^2 - AC > 0$: Hyperbolic type $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$
(Wave equation, etc.)

Examples of Elliptic PDEs

- Hamiltonian and Momentum constraints

$$\begin{aligned}
\tilde{\Delta}\psi - \frac{1}{8}\psi\tilde{R} - \frac{1}{12}\psi^5 K^2 + \frac{1}{8}\psi^{-7}\tilde{A}_{ij}\tilde{A}^{ij} &= -\frac{\kappa}{8}\psi^5\rho, \\
\tilde{\Delta}W_i + \frac{1}{3}\tilde{\nabla}_i\left(\tilde{\nabla}_j W^j\right) + \tilde{R}_{ij}W^j &= \frac{2}{3}\psi^6\tilde{\nabla}_i K + \kappa\psi^{10} j_i.
\end{aligned}$$

- Apparent Horizon Finder

$$h_{,\theta\theta} + \frac{\cos\theta}{\sin\theta}h_{,\theta} + \frac{1}{\sin^2\theta}h_{,\phi\phi} - h = S(\theta,\phi).$$

- Part of Shrödinger equation with potential

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}r^2} + \left(\omega^2 - V\right)\Psi = 0.$$

- Pulsar equation

$$\left(1 - R^2\Omega_F^2\right)\left[\partial_R^2\Psi - \frac{1}{R}\partial_R\Psi + \partial_z^2\Psi\right] - 2R\Omega_F^2\partial_R\Psi + 16\pi^2 I_P\frac{\mathrm{d}I_P}{\mathrm{d}\Psi} = 0.$$

Analytical methods

Simple example

- Let us consider static electromagnetic fields.
- $\vec{\nabla} \cdot \vec{E} = 4\pi\rho$ or $\nabla_i E^i = 4\pi\rho$.
- Electric field can be described with electric potential as $\vec{E} = -\vec{\nabla}\Phi$.

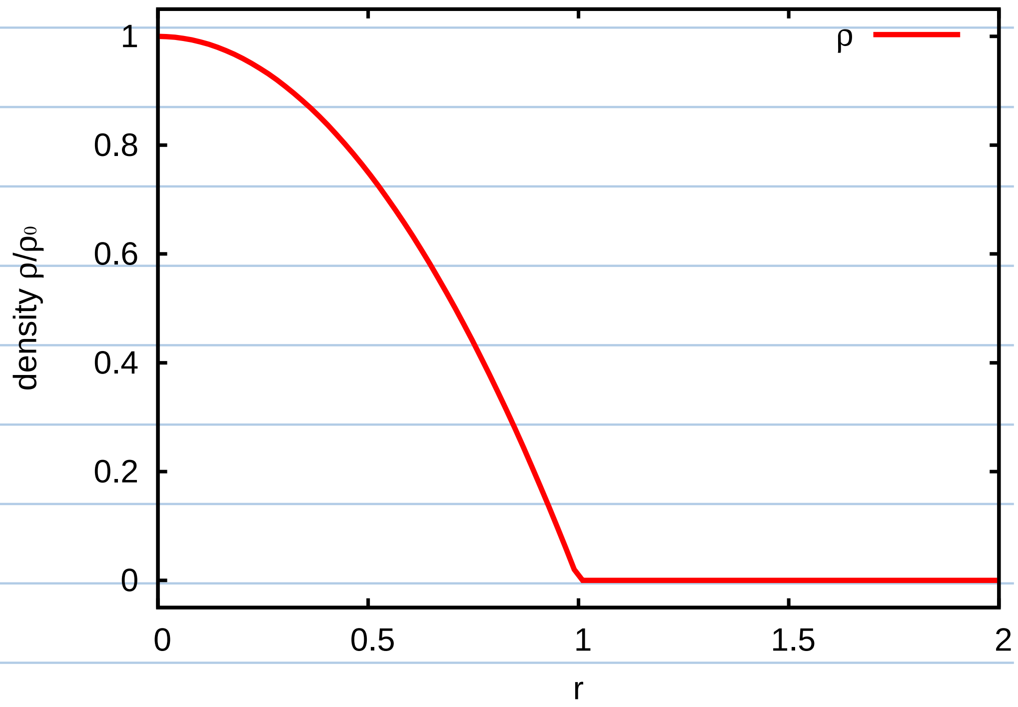
Poisson equation

$$\triangle\Phi = -4\pi\rho$$

Example of electric source

- Spherical symmetry
- Very simple problem

$$\rho(r) = \begin{cases} \rho_0 \left(1 - r^2\right), & r < 1 \\ 0, & r \geq 1 \end{cases}$$



Electric source is confined to the sphere$(r \leq 1)$.

3D spherically symmetric problem

$$\triangle\Phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}\right]\Phi + \frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right]\Phi + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Phi = -4\pi\rho$$

(i) $r \le 1$

$$\begin{aligned}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\Phi &= -4\pi\rho_0\left(1-r^2\right)\\ r^2\frac{\partial}{\partial r}\Phi &= -4\pi\rho_0\left(\frac{1}{3}r^3-\frac{1}{5}r^5+C_1\right)\\ \Phi &= -2\pi\rho_0\left(\frac{1}{3}r^2-\frac{1}{10}r^4\right)+C_2\end{aligned}$$

$C_1 = 0$ because of B.C. $E(0) = 0$.

(ii) $r > 1$

$$\begin{aligned}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\Phi &= 0\\ r^2\frac{\partial}{\partial r}\Phi &= C_3\\ \Phi &= -\frac{C_3}{r}+C_4\end{aligned}$$

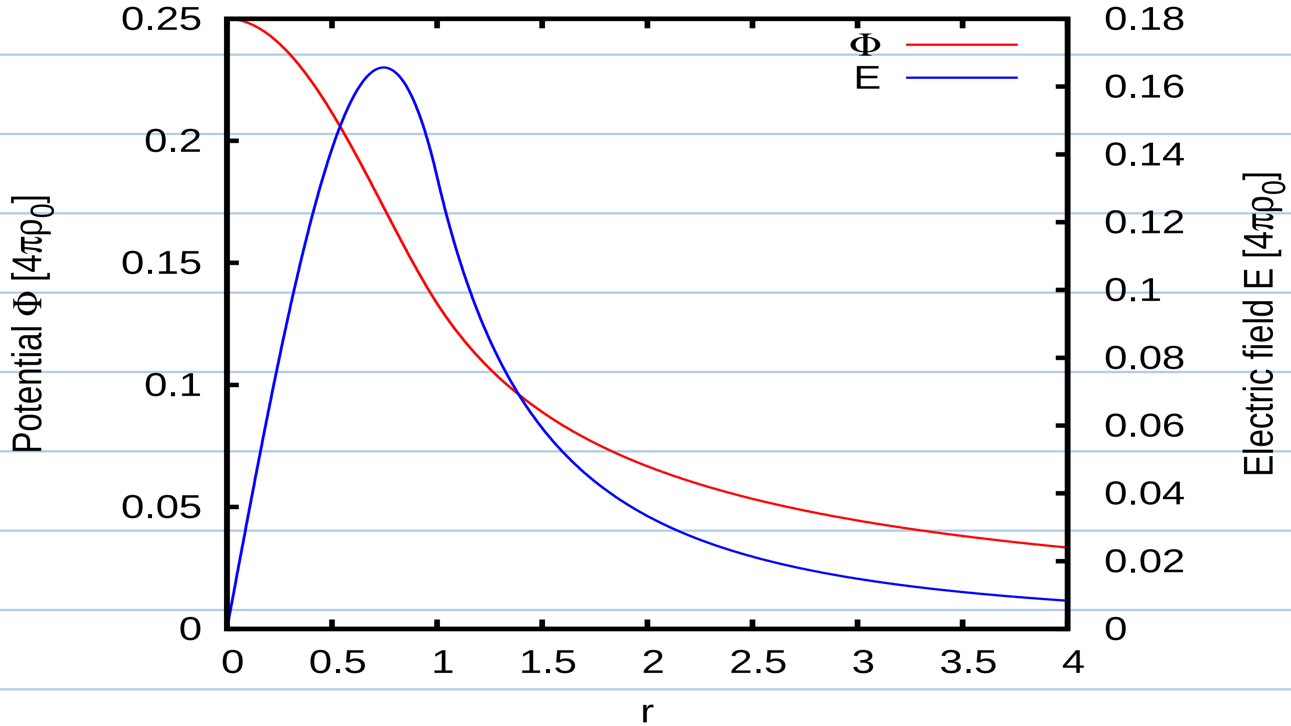
$C_4 = 0$ because of B.C. $\Phi\mid_\infty \to 0$.

(iii) Electric potential and field should be continuous at $r = 1$

$$\begin{aligned}C_3 &= -\frac{8\pi\rho_0}{15},\\ C_2 &= \pi\rho_0.\end{aligned}$$

$$\Phi(r) = \begin{cases}\pi\rho_0\left[\dfrac{r^4}{5}-\dfrac{2r^2}{3}+1\right], & r < 1\\ \dfrac{8\pi\rho_0}{15r}, & r \ge 1\end{cases}$$

Analytical Solution



Other useful analytical methods:

- with special functions(Harmonic functions, etc.),
- with Green's function,
- with Fourier transformation, $\cdots$

Numerical methods

Methods for solving elliptic PDEs

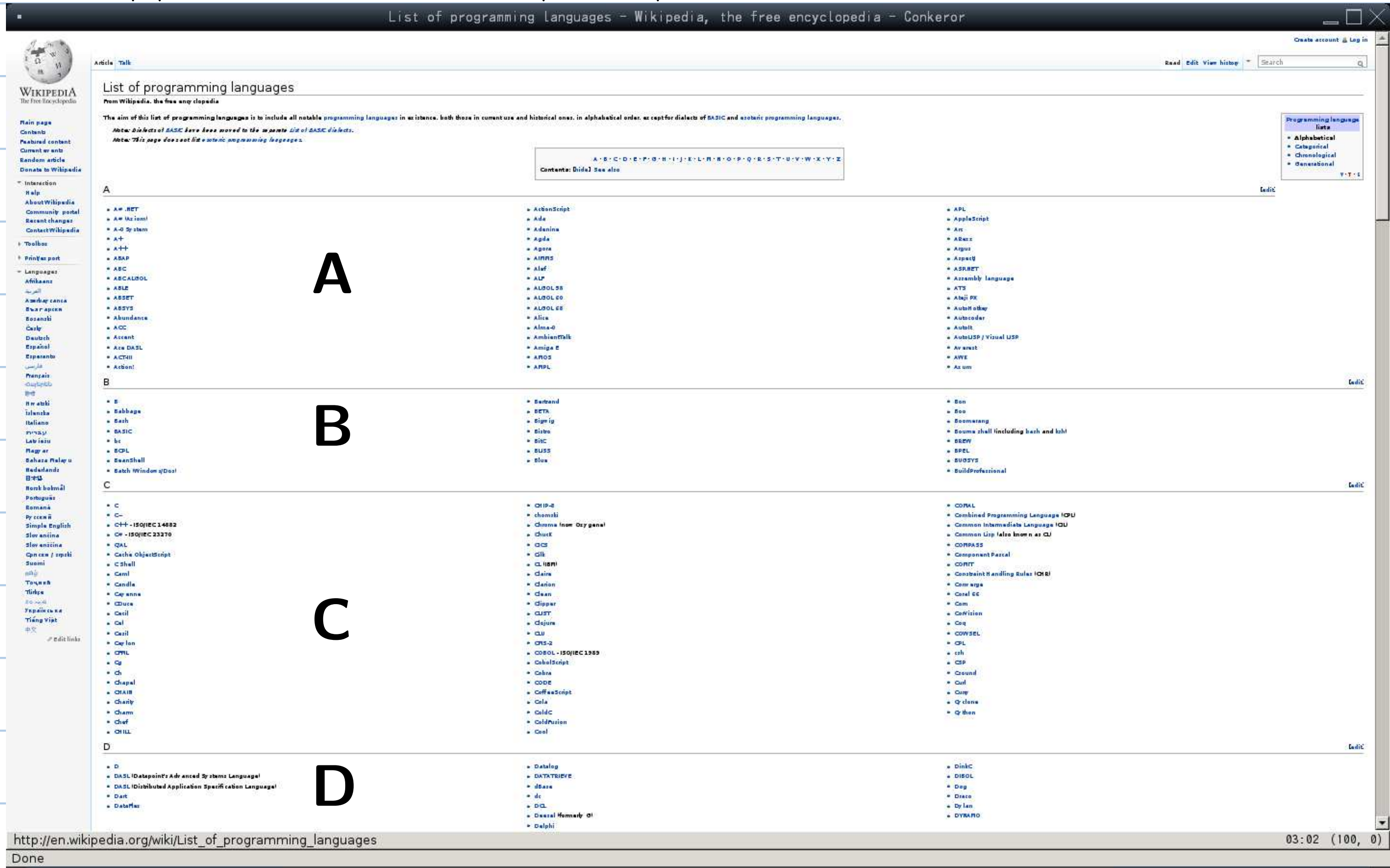
- **Relaxation method**
- **Jacobi method**
- **Gauss-Seidel method**
- **SOR method**
- Shooting method
- Conjugate Gradient(CG) method
- Spectral method
- Multi-grid method

© We really have various numerical methods to solve elliptic PDEs.

© We can also choose the programming language which we use.

Programming Languages

http://en.wikipedia.org/wiki/List_of_programming_languages



Daily Life	Shell(bash, zsh)
Physics	C++(COSMOS) Fortran90(SACRA)
Data Formatting	awk, Perl
Web	javascript, Java

Whitespace

- A programming language which accepts only white space characters(spaces, tabs, newlines)!?
  http://compsoc.dur.ac.uk/whitespace/

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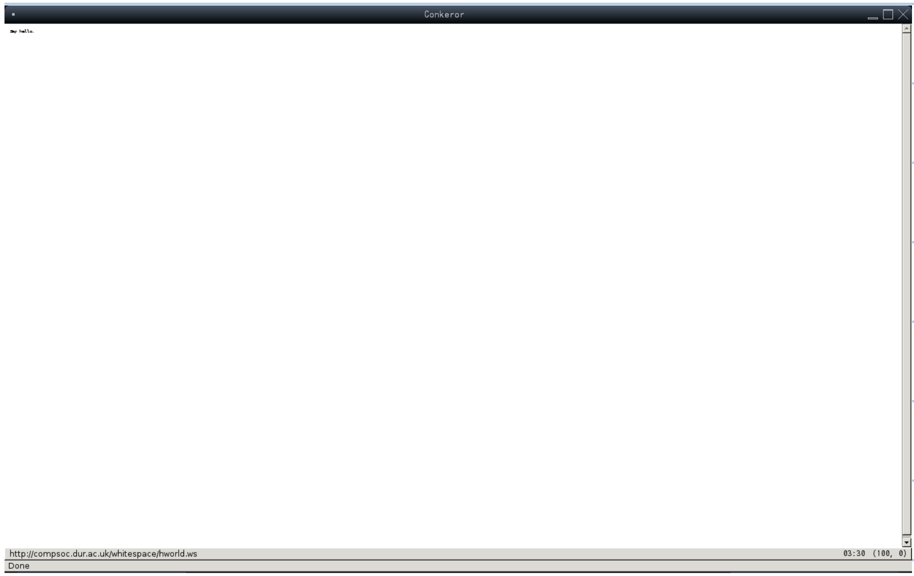

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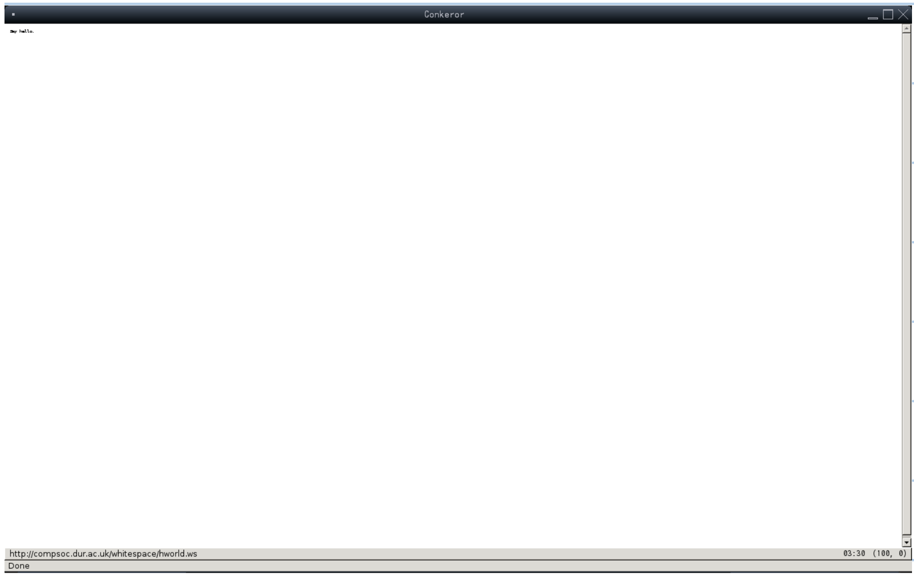

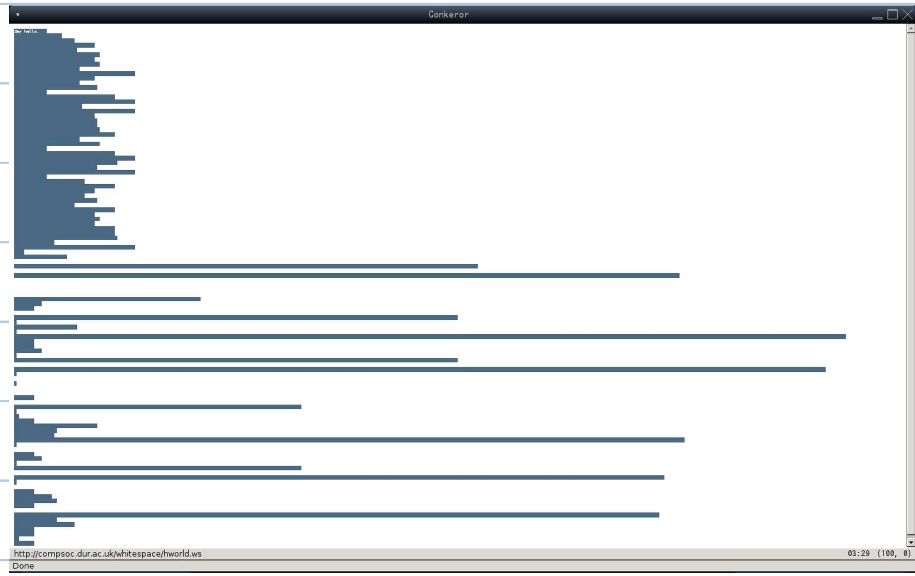

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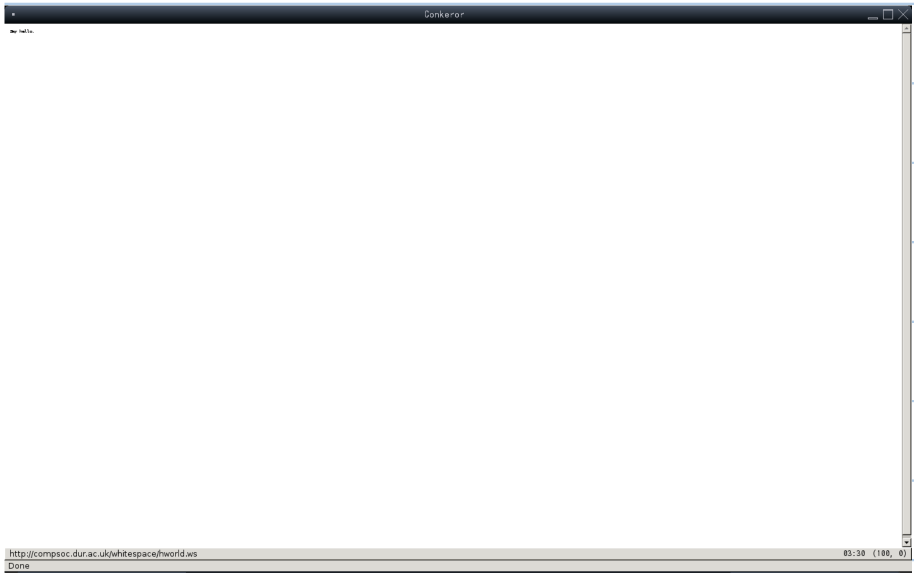
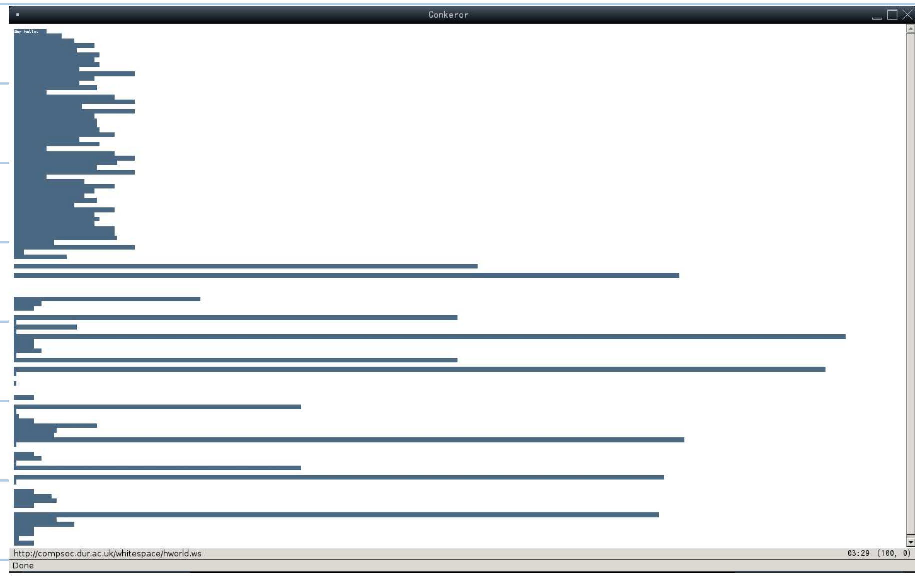


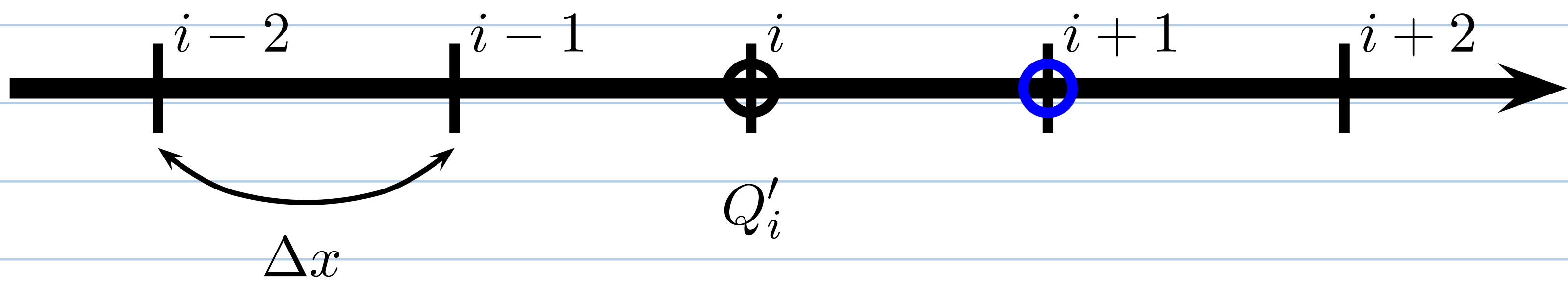


@ When we print out source code, it would be "white".
@ It will be more difficult to debug our code.
@ You had better use the code you can see more.

Difference method

Taylor expansion for forward difference

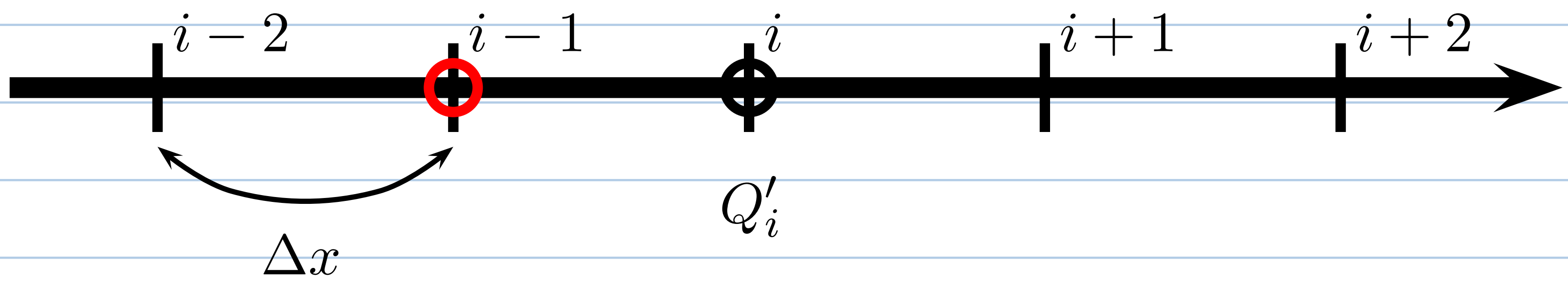
$$
\begin{aligned}
Q(x+\Delta x) &= Q(x) + \Delta x \frac{\partial Q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} + \frac{\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \mathcal{O}(\Delta x^4), \\
\frac{\partial Q}{\partial x}(x) &= \frac{1}{\Delta x}\left[\underline{Q(x+\Delta x)} - \underline{Q(x)}\right] + \mathcal{O}(\Delta x).
\end{aligned}
$$



Difference method

Taylor expansion for backward difference

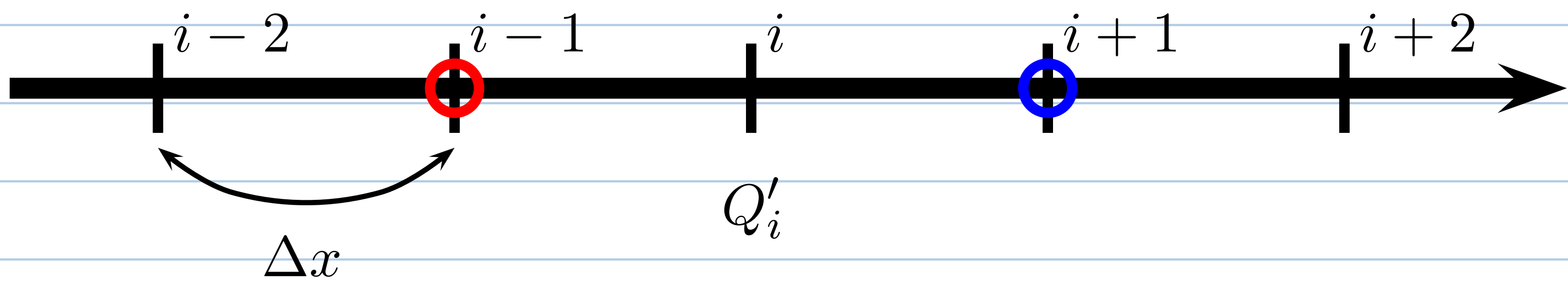
$$
\begin{aligned}
Q(x-\Delta x) &= Q(x) - \Delta x \frac{\partial Q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} - \frac{\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \mathcal{O}(\Delta x^4), \\
\frac{\partial Q}{\partial x}(x) &= \frac{1}{\Delta x}\left[\underline{Q(x)} - \underline{Q(x-\Delta x)}\right] + \mathcal{O}(\Delta x).
\end{aligned}
$$



Difference method

Taylor expansion for central difference

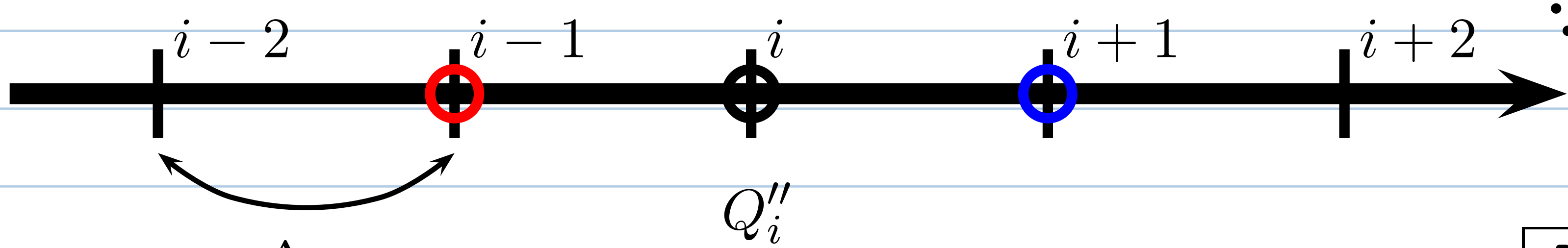
$$
\begin{aligned}
Q(x+\Delta x) &= Q(x) + \Delta x \frac{\partial Q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} + \frac{\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \mathcal{O}(\Delta x^4),\\
Q(x-\Delta x) &= Q(x) - \Delta x \frac{\partial Q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} - \frac{\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \mathcal{O}(\Delta x^4),\\
\frac{\partial Q}{\partial x}(x) &= \frac{1}{2\Delta x}\left[\underline{Q(x+\Delta x)} - \underline{Q(x-\Delta x)}\right] + \mathcal{O}(\Delta x^2).
\end{aligned}
$$



Difference method

Taylor expansion for central difference

$$
\begin{aligned}
Q(x+\Delta x) &= Q(x) + \Delta x \frac{\partial Q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} + \frac{\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \mathcal{O}(\Delta x^4),\\
Q(x-\Delta x) &= Q(x) - \Delta x \frac{\partial Q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} - \frac{\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \mathcal{O}(\Delta x^4),\\
\frac{\partial Q}{\partial x}(x) &= \frac{1}{2\Delta x}\left[Q(x+\Delta x) - Q(x-\Delta x)\right] + \mathcal{O}(\Delta x^2).
\end{aligned}
$$

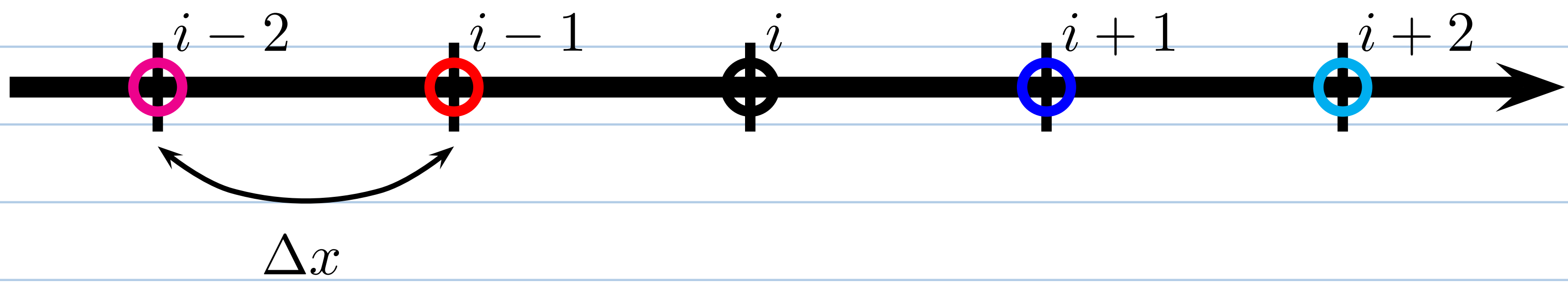


Accuracy

$$
\frac{\partial^2 Q}{\partial x^2}(x) = \frac{1}{\Delta x^2}\left[Q(x+\Delta x) - 2Q(x) + Q(x-\Delta x)\right] + \mathcal{O}(\Delta x^2).
$$

4th order

$$
\begin{aligned}
Q(x+\Delta x) &= Q(x) + \Delta x \frac{\partial Q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} + \frac{\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \frac{\Delta x^4}{24}\frac{\partial^4 Q}{\partial x^4} + \frac{\Delta x^5}{120}\frac{\partial^5 Q}{\partial x^5} + \mathcal{O}(\Delta x^6),\\
Q(x-\Delta x) &= Q(x) - \Delta x \frac{\partial Q}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} - \frac{\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \frac{\Delta x^2}{24}\frac{\partial^4 Q}{\partial x^4} - \frac{\Delta x^3}{120}\frac{\partial^5 Q}{\partial x^5} + \mathcal{O}(\Delta x^6),\\
Q(x+2\Delta x) &= Q(x) + \Delta x \frac{\partial Q}{\partial x} + \frac{2^2\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} + \frac{2^3\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \frac{2^4\Delta x^4}{24}\frac{\partial^4 Q}{\partial x^4} + \frac{2^5\Delta x^5}{120}\frac{\partial^5 Q}{\partial x^5} + \mathcal{O}(\Delta x^6),\\
Q(x-2\Delta x) &= Q(x) - \Delta x \frac{\partial Q}{\partial x} + \frac{2^2\Delta x^2}{2}\frac{\partial^2 Q}{\partial x^2} - \frac{2^3\Delta x^3}{6}\frac{\partial^3 Q}{\partial x^3} + \frac{2^4\Delta x^4}{24}\frac{\partial^4 Q}{\partial x^4} - \frac{2^5\Delta x^5}{120}\frac{\partial^5 Q}{\partial x^5} + \mathcal{O}(\Delta x^6),\\
\frac{\partial Q}{\partial x}(x) &= \frac{1}{12\Delta x}\left[-Q(x+2\Delta x) + 8Q(x+\Delta x) - 8Q(x-\Delta x) + Q(x-2\Delta x)\right] + \mathcal{O}(\Delta x^4),\\
\frac{\partial^2 Q}{\partial x^2}(x) &= \frac{1}{12\Delta x^2}\left[-Q(x+2\Delta x) + 16Q(x+\Delta x) - 30Q(x) + 16Q(x-\Delta x) - Q(x-2\Delta x)\right] + \mathcal{O}(\Delta x^4).
\end{aligned}
$$



We can use many grid points for getting high accuracy.

Relaxation method

Poisson equation

$$\Delta\psi - S = 0 \quad \Longrightarrow \quad \frac{\partial\psi}{\partial\tau} = \Delta\psi - S$$

τ : virtual time(step)

Discretization in Cartesian coordinates

$$\frac{\psi^{n+1}_{j,k,l} - \psi^{n}_{j,k,l}}{\Delta\tau} = \frac{\psi^{n}_{j+1,k,l} - 2\psi^{n}_{j,k,l} + \psi^{n}_{j-1,k,l}}{\Delta x^2} + \frac{\psi^{n}_{j,k+1,l} - 2\psi^{n}_{j,k,l} + \psi^{n}_{j,k-1,l}}{\Delta y^2} + \frac{\psi^{n}_{j,k,l+1} - 2\psi^{n}_{j,k,l} + \psi^{n}_{j,k,l-1}}{\Delta z^2} - S_{j,k,l}$$

Next step values are determined by

$$\psi^{n+1}_{j,k,l} = \left[1 - \frac{2\Delta\tau}{\Delta x^2} - \frac{2\Delta\tau}{\Delta y^2} - \frac{2\Delta\tau}{\Delta z^2}\right]\psi^{n}_{j,k,l} + \Delta\tau\left[\frac{\psi^{n}_{j+1,k,l} + \psi^{n}_{j-1,k,l}}{\Delta x^2} + \frac{\psi^{n}_{j,k+1,l} + \psi^{n}_{j,k-1,l}}{\Delta y^2} + \frac{\psi^{n}_{j,k,l+1} + \psi^{n}_{j,k,l-1}}{\Delta z^2} - S_{j,k,l}\right].$$

Repeat this iteration until $\psi^{n+1}_{j,k,l} \sim \psi^{n}_{j,k,l}$.

Jacobi method

1D Poisson equation(not spherical)

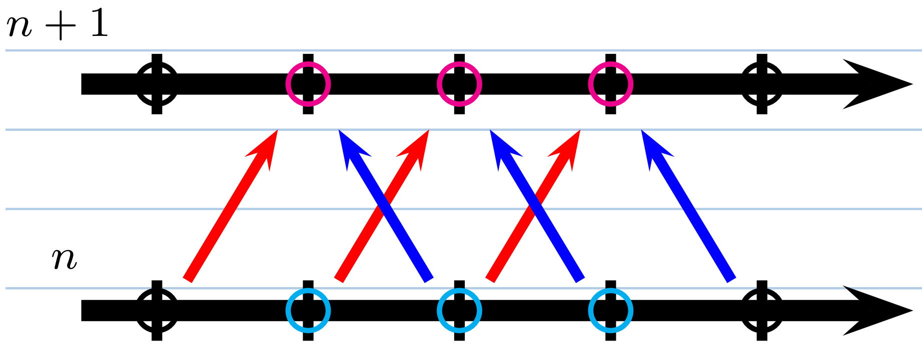
$$\Delta\psi = \frac{\partial^2\psi}{\partial x^2} = S$$

Discretization

$$\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta x^2} = S_j$$

How to update data

$$\psi_j^{n+1} = \frac{1}{2}\left[\underline{\psi_{j+1}^n} + \underline{\psi_{j-1}^n} - \Delta x^2 S_j^n\right]$$



Jacobi method

1D Poisson equation(not spherical)

$$\triangle\psi = \frac{\partial^2\psi}{\partial x^2} = S$$

2D Poisson equation

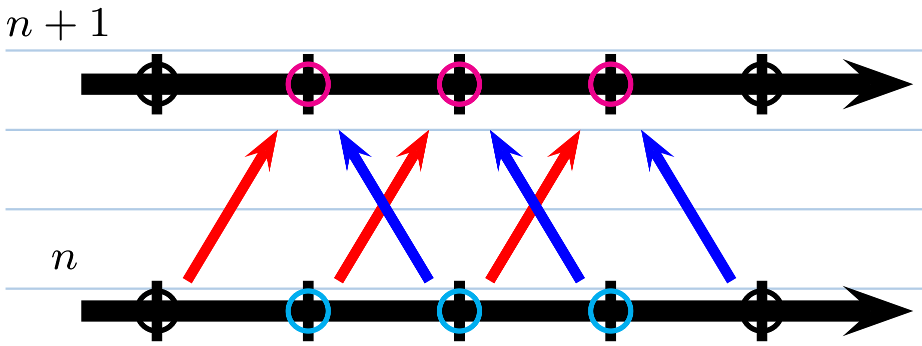
$$\triangle\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = S$$

Discretization

$$\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta x^2} = S_j$$

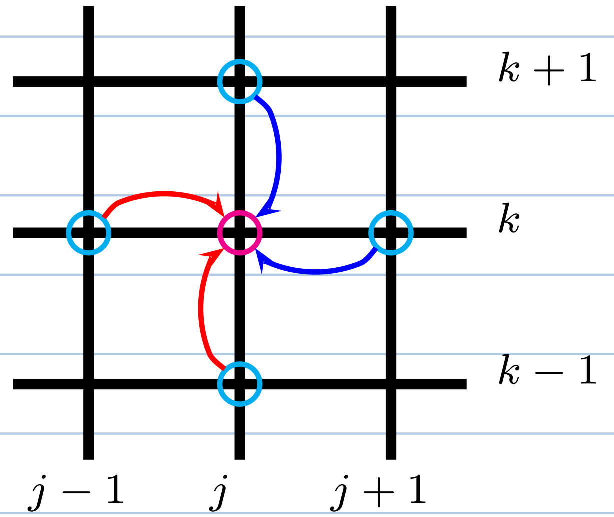
How to update data

$$\psi_j^{n+1} = \frac{1}{2}\left[\psi_{j+1}^n + \psi_{j-1}^n - \Delta x^2 S_j^n\right]$$



How to update data

$$\psi_{j,k}^{n+1} = \frac{1}{4}\left[\psi_{j+1,k}^n + \psi_{j-1,k}^n + \psi_{j,k+1}^n + \psi_{j,k-1}^n - \Delta h^2 S_{j,k}^n\right]$$



Matrix expression for Jacobi method

Discretized Poisson equation

$$\psi_{j+1} - 2\psi_j + \psi_{j-1} = \Delta x^2 S_j$$

Matrix expression

$$A_{\ell m}\psi_m = b_\ell$$

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1N} \\ 1 & -2 & 1 & \cdots & A_{2N} \\ 0 & 1 & -2 & \cdots & A_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN} \end{bmatrix} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix} = \begin{bmatrix} b_0 \\ \Delta x^2 S_1 \\ \Delta x^2 S_2 \\ \vdots \\ b_N \end{bmatrix}$$

$\boxed{\text{Jacobi method}}$ $\Longleftrightarrow$ $$\psi_j^{n+1} = \frac{1}{A_{jj}}\left[b_j - \sum_{i\neq j}^{N} A_{ji}\psi_i^n\right]$$

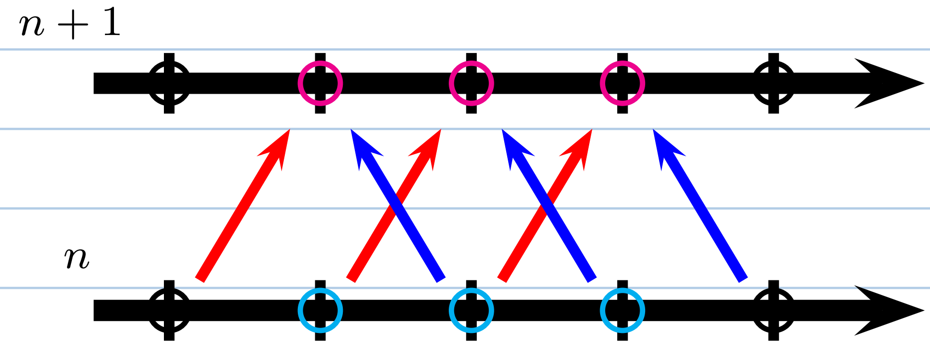
There are many methods for solving $A\vec{\psi} = \vec{b}$ as $\vec{\psi} = A^{-1}\vec{b}$.

Gauss-Seidel method

Jacobi method

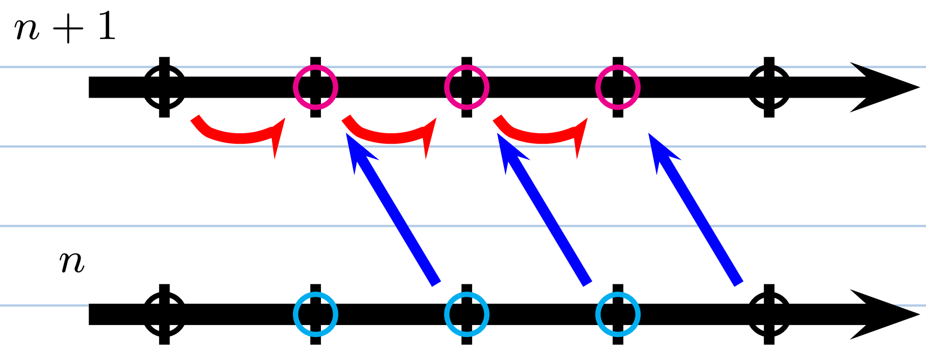
- Next step value is determined by previous step value.
- Iteration continues until values converge.

$$\psi_j^{n+1} = \frac{1}{2}\left[\underline{\psi_{j+1}^{n}} + \underline{\psi_{j-1}^{n}} - \Delta x^2 S_j^n\right]$$



Gauss-Seidel method

$$\psi_j^{n+1} = \frac{1}{2}\left[\underline{\psi_{j+1}^{n}} + \underline{\psi_{j-1}^{n+1}} - \Delta x^2 S_j^n\right]$$

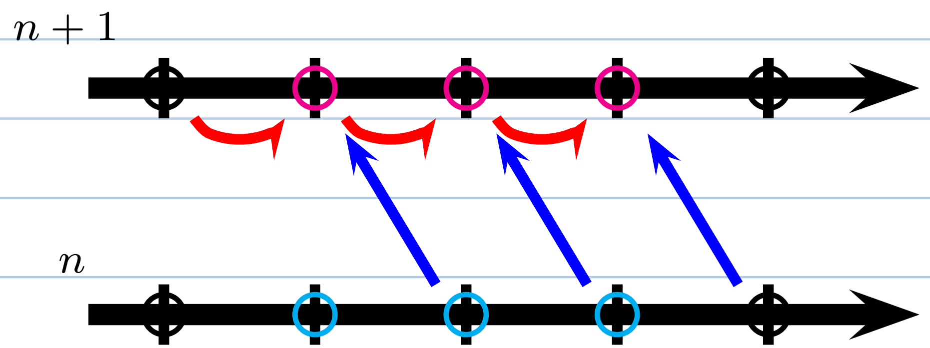


- Next step value is determined by previous step value and updated value.

SOR method

Gauss-Seidel method

$$\psi_j^{n+1,GS} = \frac{1}{2}\left[\underline{\psi_{j+1}^{n}} + \underline{\psi_{j-1}^{n+1}} - \Delta x^2 S_j^n\right]$$



Successive Over-Relaxation method

$$\triangle \equiv \psi_j^{n+1,GS} - \psi_j^n$$

$\triangle$: Amount of variation

$$\boxed{\psi_j^{n+1} = \psi_j^n + \omega\triangle}$$

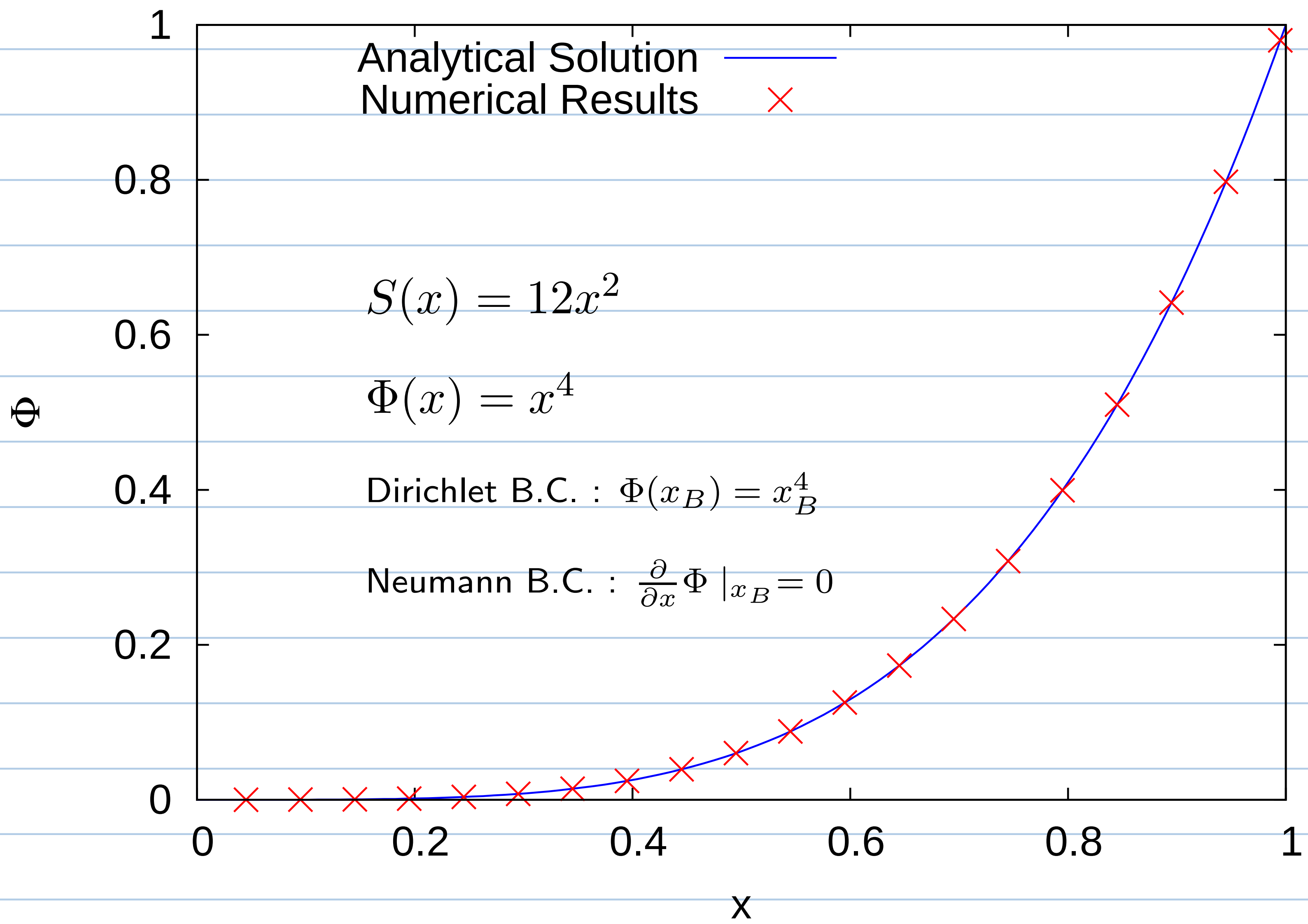
ω : Acceleration parameter

Acceleration parameter is usually chosen as $1 < \omega < 2$.

$\omega = 1$: Gauss-Seidel method

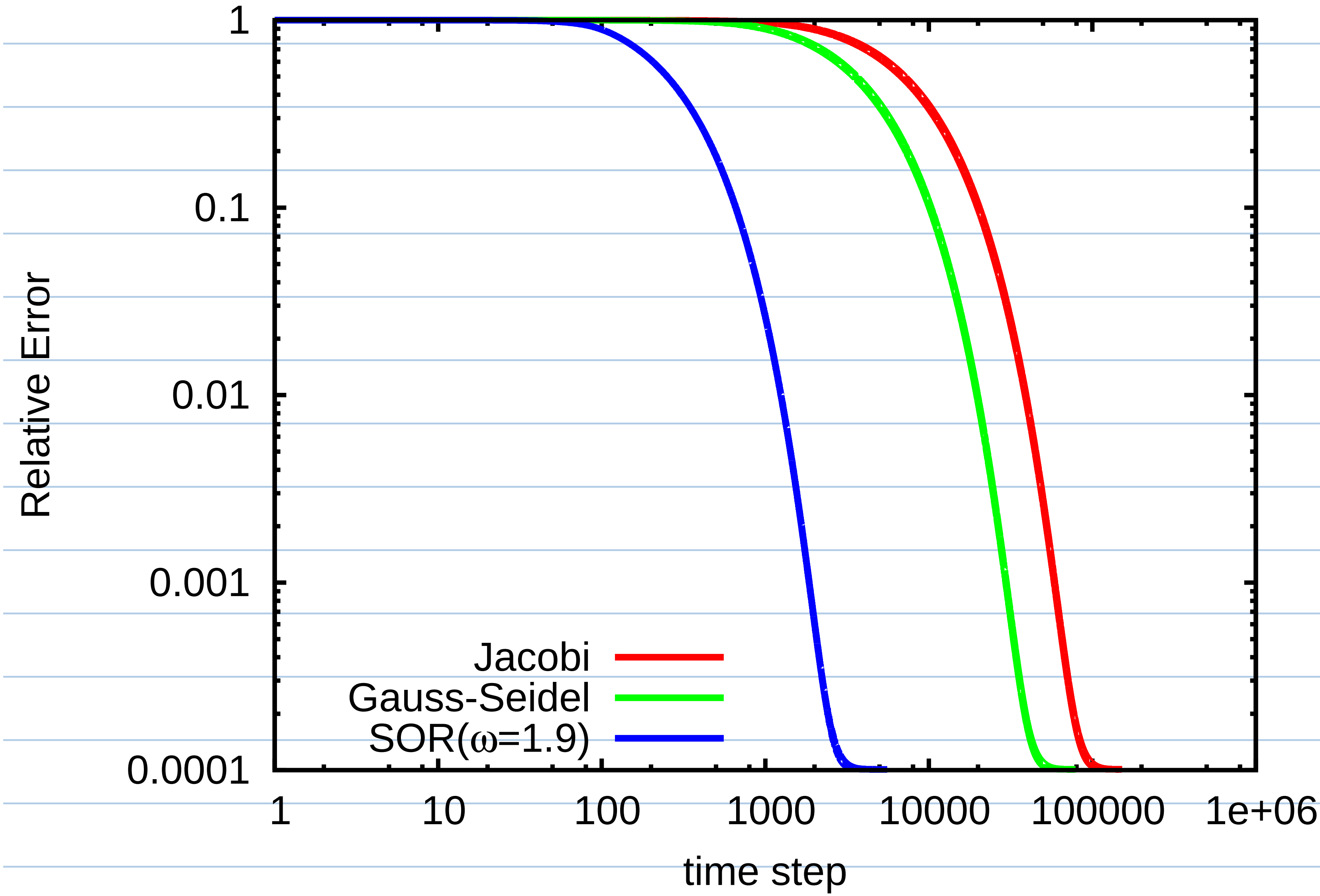
Code Tests

Test source



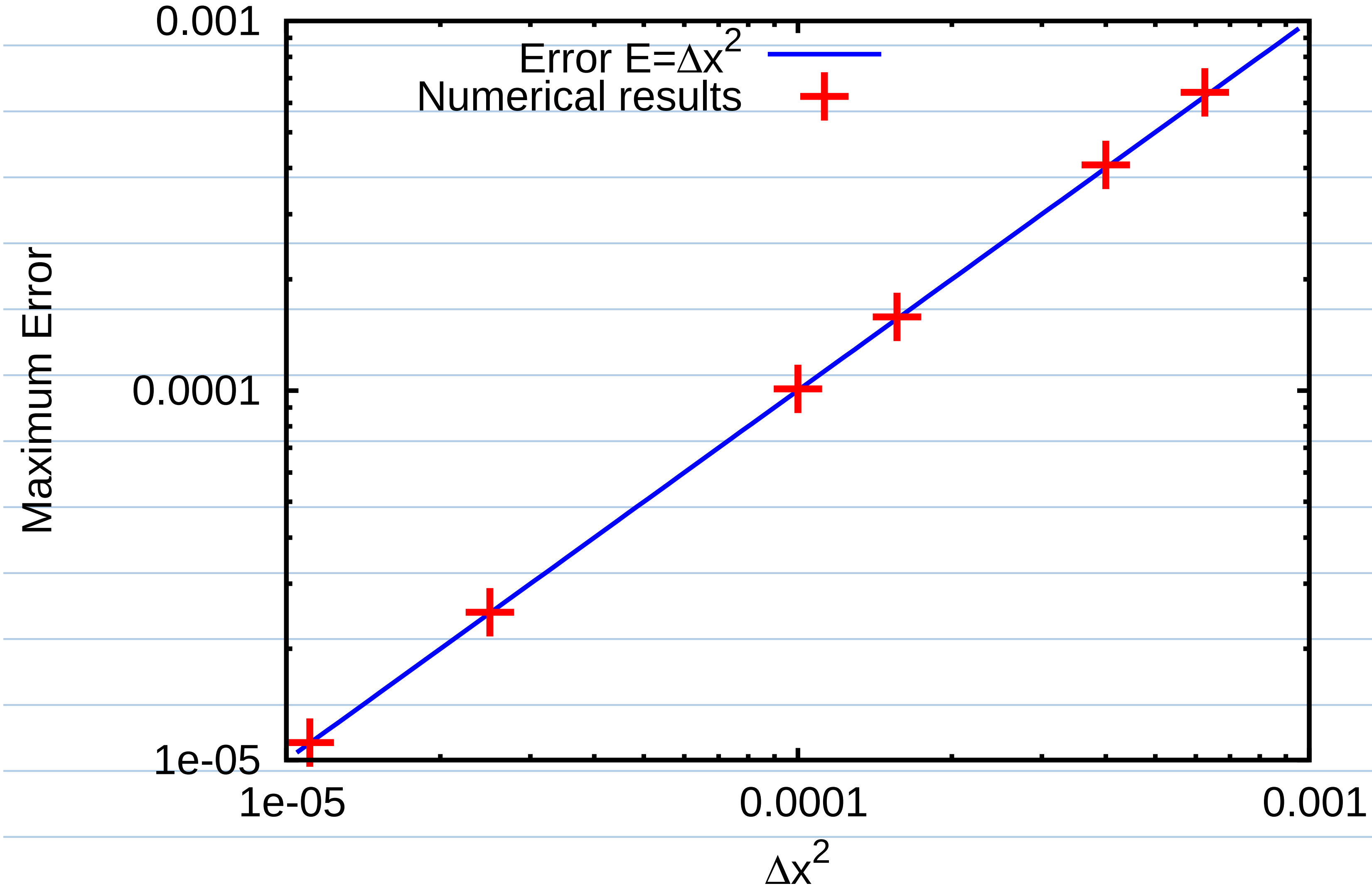
Analytical Solution
Numerical Results
$S(x) = 12x^2$
$\Phi(x) = x^4$
Dirichlet B.C. : $\Phi(x_B) = x_B^4$
Neumann B.C. : $\frac{\partial}{\partial x}\Phi\,|_{x_B} = 0$
Φ
x
0
0.2
0.4
0.6
0.8
1

Difference among methods



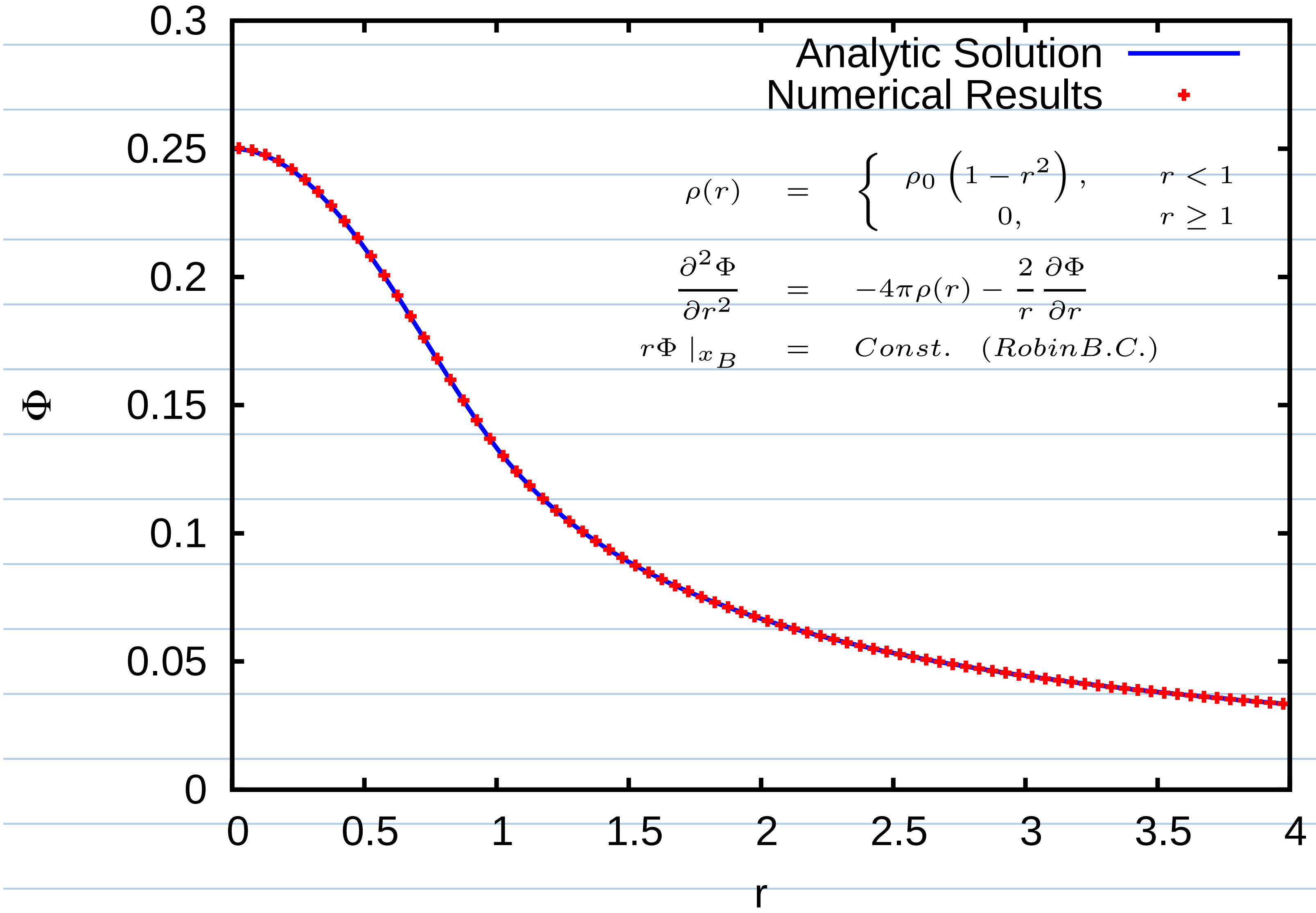
We can save the time by SOR.

Convergence Test



Convergence tests always tell the truth.

Nonlinear Source



Summary

- We have many elliptic PDEs in physics.
- Sometimes, we can solve it analytically, but in general we cannot.
- It's important to know how to numerically solve it.
- I reviewed how to solve elliptic PDEs.
- I made codes, showed test results and will upload these with some exercises.
- With these codes, you only have to change boundary conditions and source term which you want to solve.